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Project Summary

Michigan Soil Vapor Extraction Remediation (MISER) Model: A Computer Program to Model Soil Vapor Extraction and Bioventing of Organic Chemicals in Unsaturated Geological Material

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Soil vapor extraction (SVE) and bioventing (BV) are proven strategies for remediation of unsaturated zone soils. Mathematical models are powerful tools that can be used to integrate and quantify the interaction of physical, chemical, and biological processes occurring in field scale SVE/BV systems. This report describes the conceptual and mathematical formulation, numerical implementation, and application of a multiphase, multicomponent, biodegradation model designed to simulate physical, chemical, and biological interactions occurring in field scale SVE and BV systems. The model, the Michigan Soil Vapor Extraction Remediation Model (MISER), is two-dimensional and may be run in a cross-sectional or axisymmetric mode. Phase and constituent mass balance equations are discretized with a standard Galerkin finite element approach using linear triangular elements. A modular, set-iterative solution algorithm is employed. Features of the model include: the ability to simulate multiphase gas and aqueous fluid flow; the simulation of multicomponent transport processes, incorporation of rate-limited interphase mass transfer for volatilization and dissolution of an entrapped organic liquid, volatilization and sorption of aqueous phase constituents, and biophase update; and the simulation of multicomponent biodegradation kinetics and microbial population dynamics. A complete description of the computer code, implementation procedures, and example SVE and BV simulations is included.

This Project Summary was developed by EPA's National Risk Management Research Laboratory's Subsurface Protection and Remediation Division, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Soil vapor extraction (SVE) and bioventing (BV) are proven and widely used remediation strategies which target the removal of volatile organic compounds (VOCs) from the unsaturated zone. SVE and BV are similar in that they both employ vadose zone wells and pumps to generate gas flow through the unsaturated zone. They differ fundamentally, however, in the mechanism of contaminant removal. SVE systems emphasize removal by contaminant volatilization and above ground recovery. BV systems are designed to maximize contaminant removal by *in situ* biodegradation, which is stimulated by oxygen enhancement in the air stream.

The efficiency and degree of success of SVE/BV technologies is controlled by a complex combination of physical, chemical, and biological factors. SVE systems characteristically exhibit diminishing removal efficiency and long term tailing behavior indicative of diffusion controlled mass transfer. Contributing factors may include flow bypassing in heterogeneous soils, rate limited volatilization and desorption, and contaminant occlusion due to water table upwelling. Biodegradation rates in BV systems can potentially be affected by a number of factors including: the soil moisture content and distribution, delivery of oxygen, availability of inorganic nutrients, and substrate concentration, which can be inhibitory at high levels or limiting under conditions of diffusion controlled desorption.

Because of the complexity of the processes influencing the performance of SVE/BV technologies, design and operation guidelines are frequently qualitative in nature, based on experience or simple design rules. Mathematical models are recognized as powerful tools that can be used to integrate and quantify the interaction of physical, chemical, and biological processes occurring in field scale SVE/BV systems. In addition to predicting potential mass removal, mathematical models can be used to explore alternative system designs and to investigate factors limiting successful remediation. Existing simulation models of SVE/BV systems vary in their focus and processes considered. Each may exhibit limitations in its applicability to field problems by focusing only on fluid flow or single phase fluid flow conditions, by neglecting biotransformation, or by failing to fully account for nonequilibrium mass transfer processes between all fluid phases, the soil matrix, and the biophase. This report describes the mathematical and numerical formulation of a two-dimensional, field scale SVE/BV simulator that incorporates processes of multiphase fluid flow, compositional constituent transport, nonequilibrium interphase mass transfer, and Monod kinetics for aerobic biodegradation. The simulator is entitled the MIchigan Soil Vapor Extraction Remediation Model, or MISER.

Conceptual Framework and Model Formulation

Three fluid phases are modeled in MISER: a mobile gas phase, a mobile aqueous phase, and an immobile residual organic liquid phase. The gas and aqueous phases can flow simultaneously in response to pressure and density gradients arising from fluid extraction or injection at wells, rainfall infiltration, or applied surface irrigation. The movement of the aqueous and gas phases is described by standard macroscopically averaged flow equations. Hysteretic behavior in the retention and relative permeability relations, including those arising from air entrapment, are neglected. Changes in the assumed immobile organic liquid saturation occur solely by interphase mass transfer. Organic liquid saturation is updated from the organic phase mass balance equation.

A compositional modeling approach is employed. The organic liquid is considered to be a mixture of a variable number of organic components. The gas phase is modeled with a composition of nitrogen (the major constituent of air), oxygen (the single elector acceptor), water vapor, volatile constituents of the organic liquid, and a single limiting nutrient (e.g., ammonia). The aqueous phase is assumed to be comprised of water, oxygen, soluble constituents of the organic liquid, and the limiting nutrient. To account for possible rate limited uptake by the microbes, the biophase is envisioned as a subset of the aqueous phase. Sorption to the soil particles is restricted to components of the organic liquid.

The transport and transformation of individual phase components is described by a general macroscopically averaged transport equation. Rate limited interphase mass transfer is modeled with a linear driving force expression. These expressions are used to model volatilization and dissolution of the entrapped organic liquid, mass exchange between the aqueous and gas phases, rate limited sorption, and rate limited transport to the biophase. Complete drying of the aqueous phase is not considered and, consequently, solid phase sorption from the vapor phase is neglected. Nonlinear sorption to the solid phase is modeled with a Freundlich isotherm.

Biodegradation is modeled solely as an aerobic process. Biodegradation is assumed to occur only within the aqueous phase by an indigenous, spatially heterogeneous, mixed microbial population that is present as attached microcolonies. It is further assumed that biomass growth does not affect soil permeability, that there is no biomass transport, and that detachment or sloughing of the attached biofilm is negligible. Monod-type kinetic expressions are employed to describe biophase utilization of substrates, electron acceptor, and a single limiting nutrient. MISER has the capability to simulate biophase uptake of substrate, oxygen, and nutrient as an equilibrium or rate limited process. MISER incorporates inhibitory effects on biokinetics resulting from the presence of excessively high or low substrate concentrations, or due to the presence of oxygen below a minimum threshold limit. Growth and decay of the attached microbial population is modeled with a Monod-type kinetic expression, extended to constrain biomass concentration between a minimum value reflecting the indigenous population present in uncontaminated subsurface environments, and a maximum permitted biomass concentration.

Numerical Development

The flow and transport equations are discretized in two space dimensions using a standard Galerkin finite element approach with linear triangular elements. The coupled nonlinear equations are solved using a modular, set-iterative solution algorithm. In this approach, the sets of flow, transport, and biodegradation equations are decoupled and solved separately. The set-iterative approach substantially reduces the size of solution matrices and enhances flexibility. With this scheme, different numerical approaches, as well as alternative grid and time discretization schemes, can potentially be applied for each equation set. The modular approach also facilitates application of the model to simplified scenarios, such as steady flow situations or SVE in the absence of biotransformations.

The flow equations are solved with a pressure based simultaneous solution scheme, using a Picard iteration scheme to account for nonlinearities. Subsequently, the entire set of constituent transport equations for the mobile aqueous and gas phases, and immobile NAPL residual and solid phases are solved sequentially using Picard iteration schemes. Mass exchange terms and molecular weights are updated at each iteration. The entire process is then repeated until convergence for all constituent concentrations in all phases is obtained. NAPL saturations and biotransformations are updated at the end of the time step.

Model Verification

Extensive verification of numerical solutions was conducted by material balance computations, comparison with analytical solutions for simplified scenarios, intermodel comparisons, and comparison with published column data.

Numerical solutions of aqueous flow were verified with analytical expressions for the one-dimensional Richards equation, and by intermodel comparison for conditions of two-dimensional axisymmetric moisture infiltration into a two layer system. Predictions of unsteady radial flow of gas were verified against one-dimensional quasi-analytical solutions which take into account nonlinearities stemming from compressibility and the Klinkenberg effect.

Numerical solutions of contaminant transport were verified against one- and two-dimensional analytical solutions for advective-dispersive transport of a single constituent subject to first order decay. Verification of biokinetics was conducted by 1) comparison with the two-dimensional analytical solutions by adjusting Monod parameters to represent first order biodegradation rates; and 2) intermodel comparison for conditions of microbial growth and degradation in a one-dimensional soil column.

Program Description and Example Simulations

MISER is developed in the FORTRAN 77 programming language and is comprised of 25 program modules. The modular format enhances clarity, facilitates logic tracing and code modification, and enables the code to be easily programmed to run in different modes. Due to the large number of equations being solved and the complexity of the solution algorithm, the code is intended to be used on work station platforms or main frame computers. A description of major code variables and a complete source code listing is provided.

Input data are organized into two main input files, one required error message file, and an optional restart file used for run continuations. Considerable parametric inputs are required to describe the physical, chemical and biological characteristics, as well as the numerical control features. A complete description of all input data and the organization of input data blocks is provided in the report.

Output formats and files are flexible. Optional output files can be generated for runtime information, material balance computations, contour plot data files, time series information, and restart information.

Example Simulations

Three example simulations are presented to illustrate application of the MISER model. Two-dimensional axisymmetric simulations are presented for hypothetical SVE and BV scenarios. The physical system is an unsaturated medium sand, intersected with a layer of slightly less permeable fine sand. Entrapped toluene liquid is present in each layer. An extraction/injection well is positioned in the center of the initial NAPL distribution, and an impervious surface cap is present on the ground surface. A listing of all input data files is included as an appendix.

Remediation of the contaminated soil by SVE was simulated by the numerical application of a constant extraction rate of 100 standard cubic feet per minute (scfm). Mass transfer coefficients were selected to represent relatively rapid organic liquid volatilization and slower rates for desorption and aqueous/gas partitioning. A temporal progression of predicted organic liquid saturation profiles illustrates the effects of organic liquid persistence in low permeability zones due to flow bypassing. Complete removal of the organic liquid occurs relatively quickly. However, due to the magnitude of the selected mass transfer coefficients, there is long term persistence of contaminant mass on the solid phase and in the pore water, producing a persistent low level of contaminant discharge at the well. In this simulation, the long term SVE efficiency is controlled by the aqueous-solid desorption rate after the period of organic liquid removal.

Remediation of the contaminated soil by BV was simulated by the numerical application of a constant injection rate of one cubic feet per minute (scfm) to supply oxygen and enhance biotransformation. Air injection produces outward radial movement of oxygen (electron acceptor), as well as toluene (substrate) due to volatilization from the organic liquid. Organic liquid removal also progresses radially outward. Similar to the SVE scenario there is substantial persistence of organic liquid within the low permeability zone due to flow bypassing. An examination of the temporal progression of the predicted growth of biomass over the course of BV simulation reveals that, due to substrate inhibition, biomass growth is concentrated along the outside edge of the organic liquid core, developing a so-called “biofence.” Once the “biofence” has developed, the predicted toluene removal from the gas phase occurs over a relatively short distance, and there is little or no growth radially outside of the “biofence” due to an absence of substrate. Biomass growth is also observed to fill in regions close to the well after organic liquid has been removed and aqueous concentrations fall below the inhibitory threshold.

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The complete report, entitled "Michigan Soil Vapor Extraction Remediation (MISER) Model: A Computer Program to Model Soil Vapor Extraction and Bioventing of Organic Chemicals in Unsaturated Geological Material," (Order No. PB98-115355; Cost: $47.00, subject to change) will be available only from:

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